Preface

The study of atomic and molecular physics embraces all aspects of contemporary human activity. It is the ancestor of all of the technologies that are used today and has paved the way for significant breakthroughs in a variety of other scientific fields. The pursuit of curiosity through investigation and the development of new understanding still gives it a place of honour apart from its primary uses. It is a large region that is home to a wide variety of ecosystems, and recent years have seen a dizzying array of significant advancements. As a branch of atomic and molecular physics, electron scattering has developed into a well-established field of study that has important applications across the scientific and technological spectrum. New experimental and computational methods have sparked renewed interest in investigating electron interactions with atomic and molecule targets in both the gaseous and condensed phases of matter. Atomic-molecular collision physics is at the forefront of cutting-edge multidisciplinary research, providing important model studies for many of the new fields of inquiry. These interactions, which can be employed as probes, play an important part in a diverse spectrum of natural processes.

Calculations of electron impacts and collisions on molecular targets that are relevant to industrial and plasma fields, biomedical research and atmospheric sciences are reported in this thesis. This thesis presents theoretical studies on molecular targets in the range of 0.1 eV to 5000 eV in which an electron collides with the target molecule and induces various elastic and inelastic interaction processes. In light of the numerous uses of relevant cross section data in a variety of different pure and practical disciplines, there has been a resurgence in interest in the present collision computations. In this thesis, we report an approach that is effective and simple while still producing desirable results. The goal is to provide an estimation for a variety of cross sections associated with electron scattering from molecules (in gaseous and condensed or aqueous phases), including total elastic cross sections (Q_{el}), total inelastic cross sections (Q_{inel}) (including ionisation, Q_{ion} and Q_{exc}), and total cross section (Q_T). The results of these calculations are then compared with the existing experimental or theoretical results.

The following is a summary of each of the six chapters that make up this thesis.

We describe the general phenomenology of the scattering event and significance of the electron collision study in the **chapter I**. Various electron collision processes taking place during the electron interactions with the target system is also described in this chapter.

Chapter II deals with the adopted theoretical formalisms for the present computations. The R-matrix approach for the low energy computations, Spherical Complex Optical Potential (SCOP) and Complex Scattering Potential-ionisation contribution (CSP-ic) formalisms for the intermediate to high energy calculations are outlined in this chapter.

Chapter III reports the theoretical calculations of the inelastic collision cross-sections for the electron interactions with the deuterated molecules and sulfuric acid. The present results find its significance in the various applied fields, such as plasma sciences, semiconductor industries, planetary sciences etc. Apart from the computations of the cross-sections, various correlation study between the target parameters and cross-sections is also reported.

Total inelastic and elastic processes are quantified for electron collisions with the nucleosides, furfural, para-benzoquinone and fluoronitriles for the energy range from ionisation threshold to 5000 eV. These results are discussed and reported in the **chapter IV**.

Chapter V describes the study of electron interactions with the aqueous DNA molecules. In this chapter we have considered the aqueous phase of the molecular target system. Various applied quantities such as, cross-sections, inelastic mean free path, mass stopping power and absorbed dose which are important tools for the DNA damage assessment.

The low energy computations are done for the fluoromethane, CH_2F_2 by employing the R-matrix formalism. The result for this study is reported in **chapter VI**. Various cross-sections are calculated, viz., momentum transfer, differential, ionisation, elastic, inelastic etc for the energy range from 0.1 eV to 5000 eV.